

# The two possible values of the chromatic number of a random graph

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## Abstract

Given  $d \in (0, \infty)$  let  $k_d$  be the smallest integer  $k$  such that  $d < 2k \log k$ . We prove that the chromatic number of a random graph  $G(n, d/n)$  is either  $k_d$  or  $k_d + 1$  almost surely.

## 1. Introduction

The classical model of random graphs, in which each possible edge on  $n$  vertices is chosen independently with probability  $p$ , is denoted by  $G(n, p)$ . This model, introduced by Erdős and Rényi in 1960, has been studied intensively in the past four decades. We refer to the books [3], [5], [11] and the references therein for accounts of many remarkable results on random graphs, as well as for their connections to various areas of mathematics. In the present paper we consider random graphs of bounded average degree, i.e.,  $p = d/n$  for some fixed  $d \in (0, \infty)$ .

One of the most important invariants of a graph  $G$  is its chromatic number  $\chi(G)$ , namely the minimum number of colors required to color its vertices so that no pair of adjacent vertices has the same color. Since the mid-1970s, work on  $\chi(G(n, p))$  has been in the forefront of random graph theory, motivating some of the field's most significant developments. Indeed, one of the most fascinating facts known [13] about random graphs is that for every  $d \in (0, \infty)$  there exists an integer  $k_d$  such that almost surely  $\chi(G(n, d/n))$  is either  $k_d$  or  $k_d + 1$ . The value of  $k_d$  itself, nevertheless, remained a mystery.

To date, the best known [12] estimate for  $\chi(G(n, d/n))$  confines it to an interval of length about  $d \cdot \frac{29 \log \log d}{2(\log d)^2}$ . In our main result we reduce this length to 2. Specifically, we prove

**THEOREM 1.** *Given  $d \in (0, \infty)$ , let  $k_d$  be the smallest integer  $k$  such that  $d < 2k \log k$ . With probability that tends to 1 as  $n \rightarrow \infty$ ,*

$$\chi(G(n, d/n)) \in \{k_d, k_d + 1\} .$$

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Indeed, we determine  $\chi(G(n, d/n))$  *exactly* for roughly half of all  $d \in (0, \infty)$ .

**THEOREM 2.** *If  $d \in [(2k-1) \log k, 2k \log k)$ , then with probability that tends to 1 as  $n \rightarrow \infty$ ,*

$$\chi(G(n, d/n)) = k + 1.$$

The first questions regarding the chromatic number of  $G(n, d/n)$  were raised in the original Erdős-Rényi paper [8] from 1960. It was only until the 1990's, though, that any progress was made on the problem. Specifically, by the mid 1970s, the expected value of  $\chi(G(n, p))$  was known up to a factor of two for the case of fixed  $p$ , due to the work of Bollobás and Erdős [6] and Grimmett and McDiarmid [10]. This gap remained in place for another decade until, in a celebrated paper, Bollobás [4] proved that for every constant  $p \in (0, 1)$ , almost surely  $\chi(G(n, p)) = \frac{n}{2 \log n} \log \left( \frac{1}{1-p} \right) (1 + o(1))$ . Łuczak [12] later extended this result to all  $p > d_0/n$ , where  $d_0$  is a universal constant.

Questions regarding the concentration of the chromatic number were first examined in a seminal paper of Shamir and Spencer [14] in the mid-80s. They showed that  $\chi(G(n, p))$  is concentrated in an interval of length  $O(\sqrt{n})$  for all  $p$  and on an interval of length 5 for  $p < n^{-1/6-\epsilon}$ . Łuczak [13] showed that, for  $p < n^{-1/6-\epsilon}$  the chromatic number is, in fact, concentrated on an interval of length 2. Finally, Alon and Krivelevich [2] extended 2-value concentration to all  $p < n^{-1/2-\epsilon}$ .

The Shamir-Spencer theorem mentioned above was based on analyzing the so-called *vertex exposure martingale*. Indeed, this was the first use of martingale methods in random graph theory. Later, a much more refined martingale argument was the key step in Bollobás' evaluation of the asymptotic value of  $\chi(G(n, p))$ . This influential line of reasoning has fuelled many developments in probabilistic combinatorics — in particular all the results mentioned above [12], [13], [2] rely on martingale techniques.

Our proof of Theorem 1 is largely analytic, breaking with more traditional combinatorial arguments. The starting point for our approach is recent progress on the theory of sharp thresholds. Specifically, using Fourier-analytic arguments, Friedgut [9] has obtained a deep criterion for the existence of sharp thresholds for random graph properties. Using Friedgut's theorem, Achlioptas and Friedgut [1] proved that the probability that  $G(n, d/n)$  is  $k$ -colorable drops from almost 1 to almost 0 as  $d$  crosses an interval whose length tends to 0 with  $n$ . Thus, in order to prove that  $G(n, d/n)$  is almost surely  $k$ -colorable it suffices to prove that  $\liminf_{n \rightarrow \infty} \Pr[G(n, d'/n) \text{ is } k\text{-colorable}] > 0$ , for some  $d' > d$ . To do that we use the second moment method, which is based on the following special case of the Paley-Zygmund inequality: for any nonnegative random variable  $X$ ,  $\Pr[X > 0] \geq (\mathbb{E}X)^2 / \mathbb{E}X^2$ .

Specifically, the number of  $k$ -colorings of a random graph is the sum, over all  $k$ -partitions  $\sigma$  of its vertices (into  $k$  “color classes”), of the indicator that  $\sigma$  is a valid coloring. To estimate the second moment of the number of  $k$ -colorings we thus need to understand the correlation between these indicators. It turns out that this correlation is determined by  $k^2$  parameters: given two  $k$ -partitions  $\sigma$  and  $\tau$ , the probability that both of them are valid colorings is determined by the number of vertices that receive color  $i$  in  $\sigma$  and color  $j$  in  $\tau$ , where  $1 \leq i, j \leq k$ .

In typical second moment arguments, the main task lies in using probabilistic and combinatorial reasoning to construct a random variable for which correlations can be controlled. We achieve this here by focusing on the number,  $Z$ , of  $k$ -colorings in which all color classes have exactly the same size. However, we face an additional difficulty, of an entirely different nature: the correlation parameter is inherently high dimensional. As a result, estimating  $\mathbb{E}Z^2$  reduces to a certain entropy-energy inequality over  $k \times k$  doubly stochastic matrices and, thus, our argument shifts to the analysis of an optimization problem over the Birkhoff polytope. Using geometric and analytic ideas we establish the desired inequality as a particular case of a general optimization principle that we formulate (Theorem 9). We believe that this principle will find further applications, for example in probability and statistical physics, as moment estimates are often characterized by similar trade-offs.

## 2. Preliminaries

We will say that a sequence of events  $\mathcal{E}_n$  occurs with high probability (w.h.p.) if  $\lim_{n \rightarrow \infty} \Pr[\mathcal{E}_n] = 1$  and with uniformly positive probability (w.u.p.p.) if  $\liminf_{n \rightarrow \infty} \Pr[\mathcal{E}_n] > 0$ . Throughout, we will consider  $k$  to be arbitrarily large but fixed, while  $n$  tends to infinity. In particular, all asymptotic notation is with respect to  $n \rightarrow \infty$ .

To prove Theorems 1 and 2 it will be convenient to introduce a slightly different model of random graphs. Let  $G(n, m)$  denote a random (multi)graph on  $n$  vertices with precisely  $m$  edges, each edge formed by joining two vertices selected uniformly, independently, and with replacement. The following elementary argument was first suggested by Luc Devroye (see [7]).

LEMMA 3. *Define*

$$u_k \equiv \frac{\log k}{\log k - \log(k-1)} < \left(k - \frac{1}{2}\right) \log k .$$

*If  $c > u_k$ , then a random graph  $G(n, m = cn)$  is w.h.p. non- $k$ -colorable.*

*Proof.* Let  $Y$  be the number of  $k$ -colorings of a random graph  $G(n, m)$ . By Markov's inequality,  $\Pr[Y > 0] \leq \mathbb{E}[Y] \leq k^n (1 - 1/k)^m$  since, in any fixed  $k$ -partition a random edge is monochromatic with probability at least  $1/k$ . For  $c > u_k$ , we have  $k(1 - 1/k)^c < 1$ , implying  $\mathbb{E}[Y] \rightarrow 0$ .  $\square$

Define

$$c_k \equiv k \log k .$$

We will prove

PROPOSITION 4. *If  $c < c_{k-1}$ , then a random graph  $G(kn, m = ckn)$  is w.u.p.p.  $k$ -colorable.*

Finally, as mentioned in the introduction, we will use the following result of [1].

THEOREM 5 (Achlioptas and Friedgut [1]). *Fix  $d^* > d > 0$ . If  $G(n, d^*/n)$  is  $k$ -colorable w.u.p.p. then  $G(n, d/n)$  is  $k$ -colorable w.h.p.*

We now prove Theorems 1 and 2 given Proposition 4.

*Proof of Theorems 1 and 2.* A random graph  $G(n, m)$  may contain some loops and multiple edges. Writing  $q = q(G(n, m))$  for the number of such blemishes we see that their removal results in a graph on  $n$  vertices whose edge set is uniformly random among all edge sets of size  $m - q$ . Moreover, note that if  $m \leq cn$  for some constant  $c$ , then w.h.p.  $q = o(n)$ . Finally, note that the edge-set of a random graph  $G(n, p = 2c/n)$  is uniformly random conditional on its size, and that w.h.p. this size is in the range  $cn \pm n^{2/3}$ . Thus, if  $A$  is any monotone decreasing property that holds with probability at least  $\theta > 0$  in  $G(n, m = cn)$ , then  $A$  must hold with probability at least  $\theta - o(1)$  in  $G(n, d/n)$  for any constant  $d < 2c$  and similarly, for increasing properties and  $d > 2c$ . Therefore, Lemma 3 implies that  $G(n, d/n)$  is w.h.p. non- $k$ -colorable for  $d \geq (2k - 1) \log k > 2u_k$ .

To prove both theorems it thus suffices to prove that  $G(n, d/n)$  is w.h.p.  $k$ -colorable if  $d < 2c_{k-1}$ . Let  $n'$  be the smallest multiple of  $k$  greater than  $n$ . Clearly, if  $k$ -colorability holds with probability  $\theta$  in  $G(n', d/n')$  then it must hold with probability at least  $\theta$  in  $G(t, d/n')$  for all  $t \leq n'$ . Moreover, for  $n \leq t \leq n'$ ,  $d/n' = (1 - o(1))d/t$ . Thus, if  $G(kn', m = ckn')$  is  $k$ -colorable w.u.p.p., then  $G(n, d/n)$  is  $k$ -colorable w.u.p.p. for all  $d < 2c$ . Invoking Proposition 4 and Theorem 5 we thus conclude that  $G(n, d/n)$  is w.h.p.  $k$ -colorable for all  $d < 2c_{k-1}$ .  $\square$

In the next section we reduce the proof of Proposition 4 to an analytic inequality, which we then prove in the remaining sections.

### 3. The second moment method and stochastic matrices

In the following we will only consider random graphs  $G(n, m = cn)$  where  $n$  is a multiple of  $k$  and  $c > 0$  is a constant. We will say that a partition of  $n$  vertices into  $k$  parts is balanced if each part contains precisely  $n/k$  vertices. Let  $Z$  be the number of balanced  $k$ -colorings. Observe that each balanced partition is a valid  $k$ -coloring with probability  $(1 - 1/k)^m$ . Thus, by Stirling's approximation,

$$(1) \quad \mathbb{E}Z = \frac{n!}{[(n/k)!]^k} \left(1 - \frac{1}{k}\right)^m = \Omega\left(\frac{1}{n^{(k-1)/2}}\right) \left[k \left(1 - \frac{1}{k}\right)^c\right]^n.$$

Observe that the probability that a  $k$ -partition is a valid  $k$ -coloring is maximized when the partition is balanced. Thus, focusing on balanced partitions reduces the number of colorings considered by only a polynomial factor, while significantly simplifying calculations. We will show that  $\mathbb{E}Z^2 < C \cdot (\mathbb{E}Z)^2$  for some  $C = C(k, c) < \infty$ . By (1) this reduces to proving

$$\mathbb{E}Z^2 = O\left(\frac{1}{n^{k-1}}\right) \left[k \left(1 - \frac{1}{k}\right)^c\right]^{2n}.$$

This will conclude the proof of Proposition 4 since  $\Pr[Z > 0] \geq (\mathbb{E}Z)^2/\mathbb{E}Z^2$ .

Since  $Z$  is the sum of  $n!/[(n/k)!]^k$  indicator variables, one for each balanced partition, we see that to calculate  $\mathbb{E}Z^2$  it suffices to consider all pairs of balanced partitions and, for each pair, bound the probability that both partitions are valid colorings. For any fixed pair of partitions  $\sigma$  and  $\tau$ , since edges are chosen independently, this probability is the  $m$ th power of the probability that a random edge is bichromatic in both  $\sigma$  and  $\tau$ . If  $\ell_{ij}$  is the number of vertices with color  $i$  in  $\sigma$  and color  $j$  in  $\tau$ , this single-edge probability is

$$1 - \frac{2}{k} + \sum_{i=1}^k \sum_{j=1}^k \left(\frac{\ell_{ij}}{n}\right)^2.$$

Observe that the second term above is independent of the  $\ell_{ij}$  only because  $\sigma$  and  $\tau$  are balanced.

Denote by  $\mathcal{D}$  the set of all  $k \times k$  matrices  $L = (\ell_{ij})$  of nonnegative integers such that the sum of each row and each column is  $n/k$ . For any such matrix  $L$  observe that there are  $n!/(\prod_{i,j} \ell_{ij}!)$  corresponding pairs of balanced partitions. Therefore,

$$(2) \quad \mathbb{E}Z^2 = \sum_{L \in \mathcal{D}} \frac{n!}{\prod_{i=1}^k \prod_{j=1}^k \ell_{ij}!} \cdot \left[1 - \frac{2}{k} + \sum_{i=1}^k \sum_{j=1}^k \left(\frac{\ell_{ij}}{n}\right)^2\right]^{cn}.$$

To get a feel for the sum in (2) observe that the term corresponding to  $\ell_{ij} = n/k^2$  for all  $i, j$ , alone, is  $\Theta(n^{-(k^2-1)/2}) \cdot [k(1 - 1/k)^c]^{2n}$ . In fact, the

terms corresponding to matrices for which  $\ell_{ij} = n/k^2 \pm O(\sqrt{n})$  already sum to  $\Theta((\mathbb{E}Z)^2)$ . To establish  $\mathbb{E}Z^2 = O((\mathbb{E}Z)^2)$  we will show that for  $c \leq c_{k-1}$  the terms in the sum (2) decay exponentially in their distance from  $(\ell_{ij}) = (n/k^2)$  and apply Lemma 6 below. This lemma is a variant of the classical Laplace method of asymptotic analysis in the case of the Birkhoff polytope  $\mathcal{B}_k$ , i.e., the set of all  $k \times k$  doubly stochastic matrices. For a matrix  $A \in \mathcal{B}_k$  we denote by  $\rho_A$  the square of its 2-norm, i.e.  $\rho_A \equiv \sum_{i,j} a_{ij}^2 = \|A\|_2^2$ . Moreover, let  $\mathcal{H}(A)$  denote the entropy of  $A$ , which is defined as

$$(3) \quad \mathcal{H}(A) \equiv -\frac{1}{k} \sum_{i=1}^k \sum_{j=1}^k a_{ij} \log a_{ij} .$$

Finally, let  $J_k \in \mathcal{B}_k$  be the constant  $\frac{1}{k}$  matrix.

LEMMA 6. Assume that  $\varphi : \mathcal{B}_k \rightarrow \mathbb{R}$  and  $\beta > 0$  are such that for every  $A \in \mathcal{B}_k$ ,

$$\mathcal{H}(A) + \varphi(A) \leq \mathcal{H}(J_k) + \varphi(J_k) - \beta(\rho_A - 1) .$$

Then there exists a constant  $C = C(\beta, k) > 0$  such that

$$(4) \quad \sum_{L \in \mathcal{D}} \frac{n!}{\prod_{i=1}^k \prod_{j=1}^k \ell_{ij}!} \cdot \exp \left[ n \cdot \varphi \left( \frac{k}{n} L \right) \right] \leq \frac{C}{n^{k-1}} \cdot \left( k^2 e^{\varphi(J_k)} \right)^n .$$

The proof of Lemma 6 is presented in Section 6.

Let  $\mathcal{S}_k$  denote the set of all  $k \times k$  row-stochastic matrices. For  $A \in \mathcal{S}_k$  define

$$\begin{aligned} g_c(A) &= -\frac{1}{k} \sum_{i=1}^k \sum_{j=1}^k a_{ij} \log a_{ij} + c \log \left( 1 - \frac{2}{k} + \frac{1}{k^2} \sum_{i=1}^k \sum_{j=1}^k a_{ij}^2 \right) \\ &\equiv \mathcal{H}(A) + c \mathcal{E}(A) . \end{aligned}$$

The heart of our analysis is the following inequality. Recall that  $c_{k-1} = (k-1) \log(k-1)$ .

THEOREM 7. For every  $A \in \mathcal{S}_k$  and  $c \leq c_{k-1}$ ,  $g_c(J_k) \geq g_c(A)$ .

Theorem 7 is a consequence of a general optimization principle that we will prove in Section 4 and which is of independent interest. We conclude this section by showing how Theorem 7 implies  $\mathbb{E}Z^2 = O((\mathbb{E}Z)^2)$  and, thus, Proposition 4.

For any  $A \in \mathcal{B}_k \subset \mathcal{S}_k$  and  $c < c_{k-1}$  we have

$$\begin{aligned} g_c(J_k) - g_c(A) &= g_{c_{k-1}}(J_k) - g_{c_{k-1}}(A) + (c_{k-1} - c) \log \left( 1 + \frac{\rho_A - 1}{(k-1)^2} \right) \\ &\geq (c_{k-1} - c) \frac{\rho_A - 1}{2(k-1)^2} , \end{aligned}$$

where for the inequality we applied Theorem 7 with  $c = c_{k-1}$  and used that  $\rho_A \leq k$  so that  $\frac{\rho_A - 1}{(k-1)^2} \leq \frac{1}{2}$ . Thus, for every  $c < c_{k-1}$  and every  $A \in \mathcal{B}_k$

$$(5) \quad g_c(A) \leq g_c(J_k) - \frac{c_{k-1} - c}{2(k-1)^2} \cdot (\rho_A - 1) .$$

Setting  $\beta = (c_{k-1} - c)/(2(k-1)^2)$  and applying Lemma 6 with  $\varphi(\cdot) = c\mathcal{E}(\cdot)$  yields  $\mathbb{E}Z^2 = O((\mathbb{E}Z)^2)$ .

One can interpret the maximization of  $g_c$  geometrically by recalling that the vertices of the Birkhoff polytope are the  $k!$  permutation matrices (each such matrix having one non-zero element in each row and column) and  $J_k$  is its barycenter. By convexity,  $J_k$  is the *maximizer* of the entropy over  $\mathcal{B}_k$  and the *minimizer* of the 2-norm. By the same token, the permutation matrices are *minimizers* of the entropy and *maximizers* of the 2-norm. The constant  $c$  is, thus, the control parameter determining the relative importance of each quantity. Indeed, it is not hard to see that for sufficiently small  $c$ ,  $g_c$  is maximized by  $J_k$  while for sufficiently large  $c$  it is not. The pertinent question is when does the transition occur, i.e., what is the smallest value of  $c$  for which the norm gain away from  $J_k$  makes up for the entropy loss. Probabilistically, this is the point where the second moment explodes (relative to the square of the expectation), as the dominant contribution stops corresponding to uncorrelated  $k$ -colorings, i.e., to  $J_k$ .

The generalization from  $\mathcal{B}_k$  to  $\mathcal{S}_k$  is motivated by the desire to exploit the product structure of the polytope  $\mathcal{S}_k$  and Theorem 7 is optimal with respect to  $c$ , up to an additive constant. At the same time, it is easy to see that the maximizer of  $g_c$  over  $\mathcal{B}_\parallel$  is *not*  $J_k$  already when  $c = u_k - 1$ , e.g.  $g_c(J_k) < g_c(A)$  for  $A = \frac{1}{k-1}J_k + \frac{k-2}{k-1}I$ . In other words, applying the second moment method to balanced  $k$ -colorings cannot possibly match the first moment upper bound.

#### 4. Optimization on products of simplices

In this section we will prove an inequality which is the main step in the proof of Theorem 7. This will be done in a more general framework since the greater generality, beyond its intrinsic interest, actually leads to a simplification over the “brute force” argument.

In what follows we denote by  $\Delta_k$  the  $k$ -dimensional simplex  $\{(x_1, \dots, x_k) \in [0, 1]^k : \sum_{i=1}^k x_i = 1\}$  and by  $S^{k-1} \subset \mathbb{R}^k$  the unit Euclidean sphere centered at the origin. Recall that  $\mathcal{S}_k$  denotes the set of all  $k \times k$  (row) stochastic matrices. For  $1 \leq \rho \leq k$  we denote by  $\mathcal{S}_k(\rho)$  the set of all  $k \times k$  stochastic matrices with 2-norm  $\sqrt{\rho}$ , i.e.,  $\mathcal{S}_k(\rho) = \{A \in \mathcal{S}_k; \|A\|_2^2 = \rho\}$ .

*Definition 8.* For  $\frac{1}{k} \leq r \leq 1$ , let  $s^*(r)$  be the unique vector in  $\Delta_k$  of the form  $(x, y, \dots, y)$  having 2-norm  $\sqrt{r}$ . Observe that

$$x = x_r \equiv \frac{1 + \sqrt{(k-1)(kr-1)}}{k} \quad \text{and} \quad y = y_r \equiv \frac{1 - x_r}{k-1} .$$

Given  $h : [0, 1] \rightarrow \mathbb{R}$  and an integer  $k > 1$  we define a function  $f : [1/k, 1] \rightarrow \mathbb{R}$  as

$$(6) \quad f(r) = h(x_r) + (k-1) \cdot h(y_r) .$$

Our main inequality provides a sharp bound for the maximum of entropy-like functions over stochastic matrices with a given 2-norm. In particular, in Section 5 we will prove Theorem 7 by applying Theorem 9 below to the function  $h(x) = -x \log x$ .

**THEOREM 9.** *Fix an integer  $k > 1$  and let  $h : [0, 1] \rightarrow \mathbb{R}$  be a continuous strictly concave function, which is six times differentiable on  $(0, 1)$ . Assume that  $h'(0^+) = \infty$ ,  $h'(1^-) > -\infty$  and  $h^{(3)} > 0$ ,  $h^{(4)} < 0$ ,  $h^{(6)} < 0$  point-wise. Given  $1 \leq \rho \leq k$ , for  $A \in \mathcal{S}_k(\rho)$  define*

$$H(A) = \sum_{i=1}^k \sum_{j=1}^k h(a_{ij}).$$

Then, for  $f$  as in (6),

$$(7) \quad H(A) \leq \max \left\{ m \cdot k h\left(\frac{1}{k}\right) + (k-m) \cdot f\left(\frac{k\rho-m}{k(k-m)}\right); 0 \leq m \leq \frac{k(k-\rho)}{k-1} \right\} .$$

To understand the origin of the right-hand side in (7), consider the following. Given  $1 \leq \rho \leq k$  and an integer  $0 \leq m \leq \frac{k(k-\rho)}{k-1}$ , let  $B_\rho(m) \in \mathcal{S}_k(\rho)$  be the matrix whose first  $m$  rows are the constant  $1/k$  vector and the remaining  $k-m$  rows are the vector  $s^*\left(\frac{k\rho-m}{k(k-m)}\right)$ . Define  $Q_\rho(m) = H(B_\rho(m))$ . Theorem 9 then asserts that  $H(A) \leq \max_m Q_\rho(m)$ , where  $0 \leq m \leq \frac{k(k-\rho)}{k-1}$  is real.

To prove Theorem 9 we observe that if  $\rho_i$  denotes the squared 2-norm of the  $i$ -th row then

$$(8) \quad \max_{A \in \mathcal{S}_k(\rho)} H(A) = \max_{(\rho_1, \dots, \rho_k) \in \rho \Delta_k} \sum_{i=1}^k \max \left\{ \hat{h}(s); s \in \Delta_k \cap \sqrt{\rho_i} S^{k-1} \right\} ,$$

where  $\hat{h}(s) = \sum_{j=1}^k h(s_j)$ . The crucial point, reflecting the product structure of  $\mathcal{S}_k$ , is that to maximize the sum in (8) it suffices to maximize  $\hat{h}$  in each row independently. The maximizer of each row is characterized by the following proposition:



PROPOSITION 10. Fix an integer  $k \geq 1$  and let  $h : [0, 1] \rightarrow \mathbb{R}$  be a continuous strictly concave function which is three times differentiable on  $(0, 1)$ . Assume that  $h'(0^+) = \infty$ , and  $h''' > 0$  point-wise. Fix  $\frac{1}{k} \leq r \leq 1$  and assume that  $s = (s_1, \dots, s_k) \in \Delta_k \cap (\sqrt{r} S^{k-1})$  is such that

$$\hat{h}(s) \equiv \sum_{i=1}^k h(s_i) = \max \left\{ \sum_{i=1}^k h(t_i); (t_1, \dots, t_k) \in \Delta_k \cap \sqrt{r} S^{k-1} \right\}.$$

Then, up to a permutation of the coordinates,  $s = s^*(r)$  where  $s^*(r)$  is as in Definition 8.

Thus, if  $\rho_i$  denotes the squared 2-norm of the  $i$ -th row of  $A \in \mathcal{S}_k$ , Proposition 10 implies that  $H(A) \leq F(\rho_1, \dots, \rho_k) \equiv \sum_{i=1}^k f(\rho_i)$ , where  $f$  is as in (6). Hence, to prove Theorem 9 it suffices to give an upper bound on  $F(\rho_1, \dots, \rho_k)$ , where  $(\rho_1, \dots, \rho_k) \in \rho \Delta_k \cap [1/k, 1]^k$ . This is another optimization problem on a symmetric polytope and had  $f$  been concave it would be trivial. Unfortunately, in general,  $f$  is not concave (in particular, it is not concave when  $h(x) = -x \log x$ ). Nevertheless, the conditions of Theorem 9 on  $h$  suffice to impart some properties on  $f$ :

LEMMA 11. Let  $h : [0, 1] \rightarrow \mathbb{R}$  be six times differentiable on  $(0, 1)$  such that  $h^{(3)} > 0$ ,  $h^{(4)} < 0$  and  $h^{(6)} < 0$  point-wise. Then the function  $f$  defined in (6) satisfies  $f^{(3)} < 0$  point-wise.

The following lemma is the last ingredient in the proof of Theorem 9 as it will allow us to make use of Lemma 11 to bound  $F$ .

LEMMA 12. Let  $\psi : [0, 1] \rightarrow \mathbb{R}$  be continuous on  $[0, 1]$  and three times differentiable on  $(0, 1)$ . Assume that  $\psi'(1^-) = -\infty$  and  $\psi^{(3)} < 0$  point-wise. Fix  $\gamma \in (0, k]$  and let  $s = (s_1, \dots, s_k) \in [0, 1]^k \cap \gamma \Delta_k$ . Then

$$\Psi(s) \equiv \sum_{i=1}^k \psi(s_i) \leq \max \left\{ m\psi(0) + (k - m)\psi\left(\frac{\gamma}{k - m}\right); m \in [0, k - \gamma] \right\}.$$

To prove Theorem 9 we define  $\psi : [0, 1] \rightarrow \mathbb{R}$  as  $\psi(x) = f\left(\frac{1}{k} + \frac{k-1}{k}x\right)$ . Lemma 11 and our assumptions on  $h$  imply that  $\psi$  satisfies the conditions of Lemma 12 (the assumption that  $h'(0^+) = \infty$  implies that  $\psi'(1^-) = -\infty$ ). Hence, applying Lemma 12 with  $\gamma = \frac{k(\rho-1)}{k-1}$  yields Theorem 9, i.e.,

$$\begin{aligned} F(A) &= \sum_{i=1}^k \psi\left(\frac{k\rho_i - 1}{k - 1}\right) \\ &\leq \max \left\{ m\psi(0) + (k - m)\psi\left(\frac{k(\rho - 1)}{(k - 1)(k - m)}\right); m \in \left[0, k - \frac{k(\rho - 1)}{k - 1}\right] \right\}. \end{aligned}$$

4.1. *Proof of Proposition 10.* When  $r = 1$  there is nothing to prove, so assume that  $r < 1$ . We begin by observing that  $s_i > 0$  for every  $i \in \{1, \dots, k\}$ . Indeed, for the sake of contradiction, we may assume without loss of generality (since  $r < 1$ ) that  $s_1 = 0$  and  $s_2 \geq s_3 > 0$ . Fix  $\varepsilon > 0$  and set

$$\mu(\varepsilon) = \frac{s_2 - s_3 + \varepsilon - \sqrt{(s_2 - s_3 - \varepsilon)^2 + 4\varepsilon(s_3 - \varepsilon)}}{2} \quad \text{and} \quad \nu(\varepsilon) = -\mu(\varepsilon) - \varepsilon .$$

Let  $v(\varepsilon) = (\varepsilon, s_2 + \mu(\varepsilon), s_3 + \nu(\varepsilon), s_4, \dots, s_k)$ . Our choice of  $\mu(\varepsilon)$  and  $\nu(\varepsilon)$  ensures that for  $\varepsilon$  small enough  $v(\varepsilon) \in \Delta_k \cap (\sqrt{r} \cdot S^{k-1})$ . Recall that, by assumption,  $h'(0) = \infty$  and  $h'(x) < \infty$  for  $x \in (0, 1)$ . When  $s_2 > s_3$  it is clear that  $|\mu'(0)| < \infty$  and, thus,  $\left. \frac{d}{d\varepsilon} \hat{h}(v(\varepsilon)) \right|_{\varepsilon=0} = \infty$ . On the other hand, when  $s_2 = s_3 = s$  it is not hard to see that

$$\left. \frac{d}{d\varepsilon} \hat{h}(v(\varepsilon)) \right|_{\varepsilon=0} = h'(0^+) - h'(s) + sh''(s) = \infty .$$

Thus, in both cases, we have  $\left. \frac{d}{d\varepsilon} \hat{h}(v(\varepsilon)) \right|_{\varepsilon=0} = \infty$  which contradicts the maximality of  $\hat{h}(s)$ .

Since  $s_i > 0$  for every  $i$  (and, therefore,  $s_i < 1$  as well), we may use Lagrange multipliers to deduce that there are  $\lambda, \mu \in \mathbb{R}$  such that for every  $i \in \{1, \dots, k\}$ ,  $h'(s_i) = \lambda s_i + \mu$ . Observe that if we let  $\psi(u) = h'(u) - \lambda u$  then  $\psi'' = h''' > 0$ , i.e.,  $\psi$  is strictly convex. It follows in particular that  $|\psi^{-1}(\mu)| \leq 2$ . Thus, up to a permutation of the coordinates, we may assume that there is an integer  $1 \leq m \leq k$  and  $a, b \in (0, 1)$  such that  $s_i = a$  for  $i \in \{1, \dots, m\}$  and  $s_i = b$  for  $i \in \{m + 1, \dots, k\}$ . Without loss of generality  $a \geq b$  (so that in particular  $a \geq 1/k$  and  $b \leq 1/k$ ). Since  $ma + (k - m)b = 1$  and  $ma^2 + (k - m)b^2 = r$ , it follows that

$$a = \frac{1}{k} + \frac{1}{k} \sqrt{\frac{k - m}{m}(kr - 1)} \quad \text{and} \quad b = \frac{1}{k} - \frac{1}{k} \sqrt{\frac{m}{k - m}(kr - 1)} .$$

(The choice of the minus sign in the solution of the quadratic equation defining  $b$  is correct since  $b \leq 1/k$ .) Define  $\alpha, \beta : [1, r^{-1}] \rightarrow \mathbb{R}$  by

$$\alpha(t) = \frac{1}{k} + \frac{1}{k} \sqrt{\frac{k - t}{t}(kr - 1)} \quad \text{and} \quad \beta(t) = \frac{1}{k} - \frac{1}{k} \sqrt{\frac{t}{k - t}(kr - 1)} .$$

Furthermore, set  $\varphi(t) = t \cdot h(\alpha(t)) + (k - t) \cdot h(\beta(t))$ , so that  $\hat{h}(s) = \varphi(m)$ .

The proof will be complete once we check that  $\varphi$  is strictly decreasing. Observe that

$$\begin{aligned} t\alpha(t) + (k - t)\beta(t) &= 1 \\ t\alpha(t)^2 + (k - t)\beta(t)^2 &= r . \end{aligned}$$

Differentiating these identities we find that

$$\begin{aligned} \alpha(t) + t\alpha'(t) - \beta(t) + (k - t)\beta'(t) &= 0 \\ \alpha(t)^2 + 2t\alpha(t)\alpha'(t) - \beta(t)^2 + 2(k - t)\beta(t)\beta'(t) &= 0 , \end{aligned}$$

implying

$$\alpha'(t) = -\frac{\alpha(t) - \beta(t)}{2t} \quad \text{and} \quad \beta'(t) = -\frac{\alpha(t) - \beta(t)}{2(k-t)} .$$

Hence,

$$\begin{aligned} \varphi'(t) &= h(\alpha(t)) - h(\beta(t)) + t\alpha'(t)h'(\alpha(t)) + (k-t)\beta'(t)h'(\beta(t)) \\ &= h(\alpha(t)) - h(\beta(t)) - \frac{\alpha(t) - \beta(t)}{2} [h'(\alpha(t)) + h'(\beta(t))] . \end{aligned}$$

Therefore, in order to show that  $\varphi'(t) < 0$ , it is enough to prove that if  $0 \leq \beta < \alpha < 1$  then

$$h(\alpha) - h(\beta) - \frac{\alpha - \beta}{2} [h'(\alpha) + h'(\beta)] < 0 .$$

Fix  $\beta$  and define  $\zeta : [\beta, 1] \rightarrow \mathbb{R}$  by  $\zeta(\alpha) = h(\alpha) - h(\beta) - \frac{\alpha - \beta}{2} [h'(\alpha) + h'(\beta)]$ . Now,

$$\zeta'(\alpha) = \frac{\alpha - \beta}{2} \left( \frac{h'(\alpha) - h'(\beta)}{\alpha - \beta} - h''(\alpha) \right) .$$

By the Mean Value Theorem there is  $\beta < \theta < \alpha$  such that

$$\zeta'(\alpha) = \frac{\alpha - \beta}{2} [h''(\theta) - h''(\alpha)] < 0,$$

since  $h''' > 0$ . This shows that  $\zeta$  is strictly decreasing. Since  $\zeta(\beta) = 0$  it follows that for  $\alpha \in (\beta, 1]$ ,  $\zeta(\alpha) < 0$ , which concludes the proof of Proposition 10.  $\square$

4.2. *Proof of Lemma 11.* If we make the linear change of variable  $z = (k-1)(kx-1)$  then our goal is to show that the function  $g : [0, (k-1)^2] \rightarrow \mathbb{R}$ , given by

$$g(z) = h\left(\frac{1}{k} + \frac{\sqrt{z}}{k}\right) + (k-1)h\left(\frac{1}{k} - \frac{\sqrt{z}}{k(k-1)}\right),$$

satisfies  $g''' < 0$  point-wise. Differentiation gives

$$\begin{aligned} 8kz^{5/2}g'''(z) &= \frac{z}{k^2} \left[ h''' \left( \frac{1}{k} + \frac{\sqrt{z}}{k} \right) - \frac{1}{(k-1)^2} h''' \left( \frac{1}{k} - \frac{\sqrt{z}}{k(k-1)} \right) \right] \\ &\quad - \frac{3\sqrt{z}}{k} \left[ h'' \left( \frac{1}{k} + \frac{\sqrt{z}}{k} \right) + \frac{1}{k-1} h'' \left( \frac{1}{k} - \frac{\sqrt{z}}{k(k-1)} \right) \right] \\ &\quad + 3 \left[ h' \left( \frac{1}{k} + \frac{\sqrt{z}}{k} \right) - h' \left( \frac{1}{k} - \frac{\sqrt{z}}{k(k-1)} \right) \right] . \end{aligned}$$

Denote  $a = \frac{\sqrt{z}}{k}$  and  $b = \frac{\sqrt{z}}{k(k-1)}$ . Then  $8kz^{5/2}g'''(z) = \psi(a) - \psi(-b)$ , where

$$\psi(t) = t^2 h''' \left( \frac{1}{k} + t \right) - 3t h'' \left( \frac{1}{k} + t \right) + 3h' \left( \frac{1}{k} + t \right) .$$

Now

$$\psi'(t) = t^2 h'''' \left( \frac{1}{k} + t \right) - t h'''' \left( \frac{1}{k} + t \right).$$

The assumptions on  $h''''$  and  $h''''$  imply that  $\psi'(t) < 0$  for  $t > 0$ , and since  $a \geq b$ , it follows that  $\psi(a) \leq \psi(b)$ . Since  $8kz^{5/2}g'''(z) = \psi(a) - \psi(-b) = [\psi(a) - \psi(b)] + [\psi(b) - \psi(-b)]$ , it suffices to show that for every  $b > 0$ ,  $\zeta(b) = \psi(b) - \psi(-b) < 0$ . Since  $\zeta(0) = 0$ , this will follow once we verify that  $\zeta'(b) < 0$  for  $b > 0$ . Observe now that  $\zeta'(\beta) = b\chi(b)$ , where

$$\chi(b) = b \left[ h'''' \left( \frac{1}{k} + b \right) + h'''' \left( \frac{1}{k} - b \right) \right] - \left[ h'''' \left( \frac{1}{k} + b \right) - h'''' \left( \frac{1}{k} - b \right) \right].$$

Our goal is to show that  $\chi(b) < 0$  for  $b > 0$ , and since  $\chi(0) = 0$  it is enough to show that  $\chi'(b) < 0$ . But

$$\chi'(b) = b \left[ h^{(5)} \left( \frac{1}{k} + b \right) - h^{(5)} \left( \frac{1}{k} - b \right) \right],$$

so that the required result follows from the fact that  $h^{(5)}$  is strictly decreasing.

4.3. *Proof of Lemma 12.* Before proving Lemma 12 we require one more preparatory fact.

LEMMA 13. *Fix  $0 < \gamma < k$ . Let  $\psi : [0, 1] \rightarrow \mathbb{R}$  be continuous on  $[0, 1]$  and three times differentiable on  $(0, 1)$ . Assume that  $\psi'(1^-) = -\infty$  and  $\psi''' < 0$  point-wise. Consider the set  $A \subset \mathbb{R}^3$  defined by*

$$A = \{(a, b, \ell) \in (0, 1] \times [0, 1] \times (0, k]; b < a \text{ and } \ell a + (k - \ell)b = \gamma\}.$$

*Define  $g : A \rightarrow \mathbb{R}$  by  $g(a, b, \ell) = \ell\psi(a) + (k - \ell)\psi(b)$ . If  $(a, b, \ell) \in A$  is such that  $g(a, b, \ell) = \max_{(a, b, \ell) \in A} g(a, b, \ell)$  then  $a = \gamma/\ell$ .*

*Proof of Lemma 13.* Observe that if  $b = 0$  or  $\ell = k$  we are done. Therefore, assume that  $b > 0$  and  $\ell < k$ . We claim that  $a < 1$ . Indeed, if  $a = 1$  then  $b = \frac{\gamma - \ell}{k - \ell} < 1$ , implying that for small enough  $\varepsilon > 0$ ,  $w(\varepsilon) \equiv \left( 1 - \varepsilon, b + \frac{\ell\varepsilon}{k - \ell}, \ell \right) \in A$ . But  $\frac{d}{d\varepsilon} g(w(\varepsilon)) \Big|_{\varepsilon=0} = -\ell\psi'(1^-) + \ell\psi'(b) = \infty$ , which contradicts the maximality of  $g(a, b, \ell)$ .

Since  $a \in (0, 1)$  and  $\ell \in (0, k)$  we can use Lagrange multipliers to deduce that there is  $\lambda \in \mathbb{R}$  such that  $\ell\psi'(a) = \lambda\ell$ ,  $(k - \ell)\psi'(b) = \lambda(k - \ell)$  and  $\psi(a) - \psi(b) = \lambda(a - b)$ . Combined, these imply

$$\psi'(a) = \psi'(b) = \frac{\psi(a) - \psi(b)}{a - b}.$$

By the Mean Value Theorem, there exists  $\theta \in (b, a)$  such that  $\psi'(\theta) = \frac{\psi(a) - \psi(b)}{a - b}$ . But, since  $\psi''' < 0$ ,  $\psi'$  cannot take the same value three times, yielding the desired contradiction.  $\square$

We now turn to the proof of Lemma 12. Let  $s \in [0, 1]^k \cap \gamma\Delta_k$  be such that  $\Psi(s)$  is maximal. If  $s_1 = \dots = s_k = 1$  then we are done, so we assume that there exists  $i$  for which  $s_i < 1$ . Observe that in this case  $s_i < 1$  for every  $i \in \{1, \dots, k\}$ . Indeed, assuming the contrary we may also assume without loss of generality that  $s_1 = 1$  and  $s_2 < 1$ . For every  $\varepsilon > 0$  consider the vector  $u(\varepsilon) = (1 - \varepsilon, s_2 + \varepsilon, s_3, \dots, s_k)$ . For  $\varepsilon$  small enough  $u(\varepsilon) \in [0, 1]^k \cap \gamma\Delta_k$ . But  $\frac{d}{d\varepsilon}\Psi(u(\varepsilon))|_{\varepsilon=0} = \infty$ , which contradicts the maximality of  $\Psi(s)$ .

Without loss of generality we can further assume that  $s_1, \dots, s_q > 0$  for some  $q \leq k$  and  $s_i = 0$  for all  $i > q$ . Consider the function  $\tilde{\Psi}(t) = \sum_{i=1}^q \psi(t_i)$  defined on  $[0, 1]^q \cap \gamma\Delta_q$ . Clearly,  $\tilde{\Psi}$  is maximal at  $(s_1, \dots, s_q)$ . Since  $s_i \in (0, 1)$  for every  $i \in \{1, \dots, q\}$ , we may use Lagrange multipliers to deduce that there is  $\lambda \in \mathbb{R}$  such that for every  $i \in \{1, \dots, q\}$ ,  $\psi'(s_i) = \lambda$ . Since  $\psi''' < 0$ ,  $\psi'$  is strictly concave. It follows in particular that the equation  $\psi'(y) = \lambda$  has at most two solutions, so that up to a permutation of the coordinates we may assume that there is an integer  $0 \leq \ell \leq q$  and  $0 \leq b < a \leq 1$  such that  $s_i = a$  for  $i \in \{1, \dots, \ell\}$  and  $s_i = b$  for  $i \in \{\ell + 1, \dots, q\}$ . Now, using the notation of Lemma 13 we have that  $(a, b, \ell) \in A$  so that

$$\begin{aligned} \Psi(s) &= (k - q)\psi(0) + g(a, b, \ell) \\ &\leq (k - q)\psi(0) + \max \left\{ \theta\psi(0) + (q - \theta)\psi \left( \frac{\gamma}{q - \theta} \right); \theta \in [0, q - \gamma] \right\} \\ &\leq \max \left\{ m\psi(0) + (k - m)\psi \left( \frac{\gamma}{k - m} \right); m \in [0, k - \gamma] \right\}. \end{aligned}$$

**5. Proof of Theorem 7**

Let  $h(x) = -x \log x$  and note that  $h'(x) = -\log x - 1$ ,  $h'''(x) = \frac{1}{x^2}$ ,  $h^{(4)}(x) = \frac{-2}{x^3}$  and  $h^{(6)}(x) = \frac{-24}{x^5}$ , so that the conditions of Theorem 9 are satisfied in this particular case. By Theorem 9 it is, thus, enough to show that for  $c \leq c_{k-1} = (k - 1) \log(k - 1)$ ,

$$\begin{aligned} (9) \quad \frac{m \log k}{k} + \frac{k - m}{k} f \left( \frac{k\rho - m}{k(k - m)} \right) + c \log \left( 1 - \frac{2}{k} + \frac{\rho}{k^2} \right) \\ \leq \log k + 2c \log \left( 1 - \frac{1}{k} \right), \end{aligned}$$

for every  $1 \leq \rho \leq k$  and  $0 \leq m \leq \frac{k(k-\rho)}{k-1}$ . Here  $f$  is as in (6) for  $h(x) = -x \log x$ .

Inequality (9) simplifies to

$$(10) \quad c \log \left( 1 + \frac{\rho - 1}{(k - 1)^2} \right) \leq \left( 1 - \frac{m}{k} \right) \left[ \log k - f \left( \frac{k\rho - m}{k(k - m)} \right) \right].$$

Setting  $t = m/k$ ,  $s = \rho - 1$  and using the inequality  $\log(1 + a) \leq a$ , it suffices to demand that for every  $0 \leq t \leq 1 - \frac{s}{k-1}$  and  $0 \leq s \leq k - 1$ ,

$$(11) \quad \frac{cs}{(k - 1)^2} \leq (1 - t) \left[ f \left( \frac{1}{k} \right) - f \left( \frac{1}{k} + \frac{s}{k(1 - t)} \right) \right].$$

To prove (11) we define  $\eta : (0, 1 - 1/k] \rightarrow \mathbb{R}$  by

$$\eta(y) = \frac{f \left( \frac{1}{k} \right) - f \left( \frac{1}{k} + y \right)}{y},$$

and  $\eta(0) = -f' \left( \frac{1}{k} \right) = \frac{k}{2}$ , making  $\eta$  continuous on  $[0, 1 - 1/k]$ . Observe that (11) reduces to

$$c \leq \frac{(k - 1)^2}{k} \cdot \eta \left( \frac{s}{k(1 - t)} \right).$$

Now,  $\eta'(y) = \frac{\zeta(y)}{y^2}$ , where  $\zeta(y) = f \left( \frac{1}{k} + y \right) - f \left( \frac{1}{k} \right) - yf' \left( \frac{1}{k} + y \right)$ . Observe that  $\zeta'(y) = -yf'' \left( \frac{1}{k} + y \right)$  so, by Lemma 11,  $\zeta$  can have at most one zero in  $(0, 1 - \frac{1}{k})$ . A straightforward computation gives that  $\zeta \left( \frac{(k-2)^2}{k(k-1)} \right) = 0$ , so  $\eta$  achieves its global minimum on  $[0, 1 - \frac{1}{k}]$  at  $y \in \left\{ 0, \frac{(k-2)^2}{k(k-1)}, 1 - \frac{1}{k} \right\}$ . Direct computation gives  $\eta \left( 1 - \frac{1}{k} \right) = \frac{k}{k-1} \cdot \log k$ ,  $\eta \left( \frac{(k-2)^2}{k(k-1)} \right) = \frac{k-1}{k-2} \cdot \log(k - 1)$  and, by definition,  $\eta(0) = \frac{k}{2}$ . Hence

$$(12) \quad \begin{aligned} \frac{(k - 1)^2}{k} \cdot \eta \left( \frac{s}{k(1 - t)} \right) &\geq \frac{(k - 1)^2}{k} \cdot \min \left\{ \frac{k}{2}, \frac{k - 1}{k - 2} \cdot \log(k - 1), \frac{k}{k - 1} \cdot \log k \right\} \\ &= \frac{(k - 1)^3}{k(k - 2)} \cdot \log(k - 1) > c_{k-1}, \end{aligned}$$

where (12) follows from elementary calculus.

*Remark.* The above analysis shows that Theorem 7 is asymptotically optimal. Indeed, let  $A$  be the stochastic matrix whose first  $k - 1$  rows are the constant  $1/k$  vector and whose last row is the vector  $s^*(r)$ , defined in Definition 8, for  $r = \frac{1}{k} + \frac{(k-2)^2}{k(k-1)}$ . This matrix corresponds to  $m = k - 1$  and  $\rho = 1 + \frac{(k-2)^2}{k(k-1)}$  in (10), and a direct computation shows that any  $c$  for which Theorem 7 holds must satisfy  $c < c_{k-1} + 1$ .

6. Appendix: Proof of Lemma 6

If  $(\ell_{ij})$  are nonnegative integers such that  $\sum_{i,j} \ell_{ij} = n$ , standard Stirling approximations imply

$$(13) \quad \frac{n!}{\prod_{i=1}^k \prod_{j=1}^k \ell_{ij}!} \leq \left[ \prod_{i=1}^k \prod_{j=1}^k \left( \frac{\ell_{ij}}{n} \right)^{-\ell_{ij}/n} \right]^n \cdot \min \left\{ 3\sqrt{n}, \left[ (2\pi n)^{k^2-1} \prod_{i=1}^k \prod_{j=1}^k \frac{\ell_{ij}}{n} \right]^{-1/2} \right\}.$$

Since  $|\mathcal{D}| \leq (n+1)^{(k-1)^2}$ , the contribution to the sum in (4) of the terms for which  $\rho_{\frac{k}{n}L} > 1 + 1/(4k^2)$  can, thus, be bounded by

$$(14) \quad 3\sqrt{n}(n+1)^{(k-1)^2} \left( e^{\mathcal{H}(\frac{k}{n}L) + \log k + \varphi(\frac{k}{n}L)} \right)^n \leq 3n^{k^2} \left( k^2 e^{\varphi(J_k)} \right)^n \cdot e^{-\frac{\beta n}{4k^2}} = O \left( n^{-k^2} \right) \left( k^2 e^{\varphi(J_k)} \right)^n.$$

Furthermore, if  $L \in \mathcal{D}$  is such that  $\rho_{\frac{k}{n}L} \leq 1 + \frac{1}{4k^2}$ , then for every  $1 \leq i, j \leq k$  we have

$$\left( \frac{k}{n} \ell_{ij} - \frac{1}{k} \right)^2 \leq \sum_{s=1}^k \sum_{t=1}^k \left( \frac{k}{n} \ell_{st} - \frac{1}{k} \right)^2 = \rho_{\frac{k}{n}L} - 1 \leq \frac{1}{4k^2}.$$

Therefore, for such  $L$  we must have  $\ell_{ij} \geq n/(2k^2)$  for every  $i, j$ . Therefore, by (13), (14) we get

$$(15) \quad \sum_{L \in \mathcal{D}} \frac{n!}{\prod_{i=1}^k \prod_{j=1}^k \ell_{ij}!} \cdot \exp \left[ n \varphi \left( \frac{k}{n} L \right) \right] \leq \frac{C(\beta, k)}{n^{(k^2-1)/2}} \cdot \left( k^2 e^{\varphi(J_k)} \right)^n \cdot \sum_{L \in \mathcal{D}} e^{-\beta n \left( \frac{k^2}{n^2} \rho_L - 1 \right)}.$$

Denote by  $M_k(\mathbb{R})$  the space of all  $k \times k$  matrices over  $\mathbb{R}$  and let  $F$  be the subspace of  $M_k(\mathbb{R})$  consisting of all matrices  $X = (x_{ij})$  for which the sum of each row and each column is 0. The dimension of  $F$  is  $(k-1)^2$ . Denote by  $B_\infty$  the unit cube of  $M_k(\mathbb{R})$ , i.e. the set of all  $k \times k$  matrices  $A = (a_{ij})$  such that  $a_{ij} \in [-1/2, 1/2]$  for all  $1 \leq i, j \leq k$ . For  $L \in \mathcal{D}$  we define  $T(L) = L - \frac{n}{k} J_k + (F \cap B_\infty)$ , i.e., the tile  $F \cap B_\infty$  shifted by  $L - \frac{n}{k} J_k$ .

LEMMA 14. For every  $L \in \mathcal{D}$ ,

$$e^{-\beta n \left( \frac{k^2}{n^2} \rho_L - 1 \right)} \leq e^{\frac{k^4 \beta}{4n}} \cdot \int_{T(L)} e^{-\frac{k^2 \beta}{2n} \|X\|_2^2} dX.$$

*Proof.* By the triangle inequality, we see that for any matrix  $X$

$$(16) \quad \left\| L - \frac{n}{k} J_k \right\|_2^2 \geq \frac{1}{2} \|X\|_2^2 - \left\| L - \frac{n}{k} J_k - X \right\|_2^2 \geq \frac{1}{2} \|X\|_2^2 - k^2 \left\| L - \frac{n}{k} J_k - X \right\|_\infty^2.$$

Thus, for  $X \in T(L)$  we have  $\|X\|_2^2 \leq 2 \left( \frac{k^2}{n^2} \rho_L - 1 \right) \left( \frac{n}{k} \right)^2 + \frac{k^2}{2}$ , since  $\left\| L - \frac{n}{k} J_k \right\|_2^2 = \left( \frac{k^2}{n^2} \rho_L - 1 \right) \left( \frac{n}{k} \right)^2$  and  $\left\| L - \frac{n}{k} J_k - X \right\|_\infty^2 \leq \frac{1}{4}$ . Therefore,

$$\begin{aligned} \int_{T(L)} e^{-\frac{k^2\beta}{2n} \|X\|_2^2} dX &\geq \int_{T(L)} e^{-\frac{k^4\beta}{4n}} \cdot e^{-\beta n \left( \frac{k^2}{n^2} \rho_L - 1 \right)} dX \\ &= e^{-\frac{k^4\beta}{4n}} \cdot e^{-\beta n \left( \frac{k^2}{n^2} \rho_L - 1 \right)} \text{vol}(F \cap B_\infty). \end{aligned}$$

It is a theorem of Vaaler [15] that for any subspace  $E$ ,  $\text{vol}(E \cap B_\infty) \geq 1$ , concluding the proof.  $\square$

Thus, to bound the second sum in (15) we apply Lemma 14 to get

$$\begin{aligned} \sum_{L \in \mathcal{D}} e^{-\beta n \left( \frac{k^2}{n^2} \rho_L - 1 \right)} &\leq e^{\frac{k^4\beta}{4n}} \sum_{L \in \mathcal{D}} \int_{T(L)} e^{-\frac{k^2\beta}{2n} \|X\|_2^2} dX \\ &\leq e^{\frac{k^4\beta}{4n}} \int_F e^{-\frac{k^2\beta}{2n} \|X\|_2^2} dX \\ &= e^{\frac{k^4\beta}{4n}} \int_{\mathbb{R}^{(k-1)^2}} e^{-\frac{k^2\beta}{2n} \|X\|_2^2} dX \\ &= e^{\frac{k^4\beta}{4n}} \left( \frac{2\pi n}{\beta k^2} \right)^{(k-1)^2/2} \end{aligned}$$

where we have used the fact that the interiors of the “tiles”  $\{T(L)\}_{L \in \mathcal{D}}$  are disjoint, that the Gaussian measure is rotationally invariant and that  $F$  is  $(k-1)^2$  dimensional.

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